FUNDAMENTAL MODELLING OF PULVERIZED COAL AND COAL-WATER SLURRY COMBUSTION IN A GAS TURBINE COMBUSTOR

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INTRODUCTION

A large portion of world energy resources is in the form of low grade coal. There is need to utilize these resources in an efficient and environmentally clean way. The specific approach under development by us is direct combustion in a multistage slagging combustor, incorporating control of NO_x, SO_x, and particulates. While experimental verification provides the ultimate proof of acceptability, there is an increasing realization that the detailed flow field computations of the combustion process can provide much of the necessary understanding and aid in the development process. A number of papers have dealt with the modelling of pulverized coal combustion in burners where flow field is predominantly two-dimensional (1-3). Many elements of this coal combustion model have been developed and validated under those conditions.

Our main interest is in the combustors where three-dimensional effects are of prime importance. An example of such a combustor is shown schematically in Fig. 1. The toroidal vortex combustor is currently under development through a DOE contract to Westinghouse and subcontract to ARL. This subscale, coal-fired, 6 MW combustor will be built and become operational in 1988. The coal fuel is mixed with preheated air, injected through a number of circumferentially-located jets oriented in the radius axis planes. The jets merge at the centerline, forming a vertically directed jet which curves around the combustor dome wall and gives rise to a toroidal shaped vortex. This vortex helps to push the particles radially outward, hit the walls through inertial separation and promote slagging. It also provides a high intensity flow mixing zone to enhance combustion product uniformity, and a primary mechanism for heat feed back to the incoming flow for flame stabilization.

Work describes the essential features of a coal combustion model which is incorporated into a three-dimensional, steady-state, two-phase, turbulent, reactive flow code. The code is a modified and advanced version of INTERN code originally developed at Imperial College which has gone through many stages of development and validation. Swithenbank et al[4-5] have reported spray combustion model results for an experimental can combustor. The code has since then been modified by and made public under a US Army program[6]. A number of code modifications and improvements have been made at ARL. The earlier version of code was written for a small CDC machine which relied on frequent disk/memory transfer and overlay features to carry the computations resulting in loss of computational speed. These limitations have now been removed. For spray applications, the fuel droplet vaporization generates gaseous fuel of uniform composition; hence the earlier formulation relied upon the use of conserved scalar approximation to reduce the number of species equations to be solved. In applications related to coal fuel, coal pyrolysis leads to the formation of at least two different gaseous fuels and a solid fuel of different composition. We have therefore removed the conserved scalar formulation for the sake of generality and easy adaptability to complex fuel situations.

Pulverized Coal Combustion Model

Combustion of pulverized coal particles is generally assumed to be a two-stage process consisting of devolatilization or pyrolysis of coal and heterogeneous char oxidation and gasification. The model adopted to describe pyrolysis is that of Kobayashi, et al.[7] This model proposes the use of two competing first order reactions to describe particle mass loss during pyrolysis. The process is described as

$$\text{DAF} \xrightarrow{k_1} \alpha_1 V_1 + (1 - \alpha_1)\, S_1$$

$$\text{DAF} \xrightarrow{k_2} \alpha_2 V_2 + (1 - \alpha_2)\, S_2 \qquad 1)$$

where V_1 and V_2 are volatiles of approximate elemental ratio C_6H_{12} and C_6H_6, and S_1 and S_2 are char residuals containing mostly C. Specifically for a dry ash free (daf) coal of the type $CH._8$, these reactions can be expressed as

$$CH._8 \xrightarrow{k_1} \frac{.4}{6} C_6H_{12} + .6\ C,$$

and 2)

$$CH._8 \xrightarrow{k_2} \frac{.8}{6} C_6H_6 + .2\ C.$$

The rate of disappearance of daf coal is given by

$$-\frac{d}{dt} m_{daf} = (k_1 + k_2)\, m_{daf} \qquad 3)$$

where m_{daf} is the mass of dry ash free coal, k_1 and k_2 are rate constants given by

$$k_1 = 3.7 \times 10^5 \times \exp(-8860/T)$$

$$k_2 = 1.46 \times 10^{13} \times \exp(-3017/T) \qquad 4)$$

It should be noted that Equation 2 leads to volatiles yield of 0.43 and 0.81 for slow and very rapid heating respectively. It is relatively easy to modify composition of volatiles to fit the experimental data for different coal ranks including their oxygen, nitrogen, and organically bound sulfur content. The devolatilization of coal is assumed to take place without change in the particle radius and leaves behind a lighter porous particle.

Char Oxidation and Gasification Model

Char gasification may be treated approximately as a three-stage process consisting of (i) diffusion of gaseous species to the surface, (ii) surface reaction, and (iii) diffusion of products to the bulk gas. Any of the processes may be a rate controlling step depending on the gas phase conditions, particle size and temperature, and particle pore structure. The model adopted is an extended version of Field[8] where surface diffusion and chemical reaction are taken into account. Three different surface reactions are included in the model, viz,

$$C + \frac{1}{2} O_2 \xrightarrow{k_3} CO,$$

$$C + CO_2 \xrightarrow{k_4} 2\ CO, \qquad 5)$$

and

$$C + H_2O \xrightarrow{k_5} CO + H_2.$$

For the sake of simplicity, it is assumed that all three reactions proceed independent of each other so that the char consumption rate is sum of individual rates. Rate of O_2 diffusion to the surface is given by

$$\frac{d}{dt} m_{O_2} = - k_D A_s (Y_{O_2}^{\infty} - Y_{O_2}^{s}) \qquad 6)$$

and the rate of O_2 consumption at the surface is given by

$$\frac{d}{dt} m_{O_2} = - k_r \cdot A_s \cdot Y_{O_2}^{\infty} \qquad 7)$$

Under quasi-steady-state, the two rates from Equations 6 and 7 balance each other and unknown quantity Y_O can be eliminated to give

$$\frac{d}{dt} m_{O_2} = - k_{eff} \cdot A_s \cdot Y_{O_2}^{\infty} \qquad 8)$$

where $k_{eff} = k_r k_D/(k_r + k_D)$. The diffusion rate k_D is related to the laminar diffusion coefficient, and the rate constants k_3 - k_5, taken from Stickler,[9] are given by

$$k_3 = 3.24 \times 10^{10} \times \exp(-14500/T),$$

$$k_4 = 5.75 \times 10^{13} \times \exp(-43200/T), \qquad 9)$$

and

$$k_5 = 6.38 \times 10^{11} \times \exp(-30300/T).$$

Heterogeneous char combustion is assumed to take place at the outer surface resulting in the removal of material from the surface at the constant particle density.

Devolatilization or blowing out of gaseous products hinders the diffusion of gas phase species to the surface. It is assumed that char oxidation does not begin until the devolatilization is complete.

Coal Water Slurry Combustion Model

The presence of water in pulverized coal either as moisture or as a slurry forming medium further complicates the modelling of coal pyrolysis processes. In general, the size distribution of coal slurry droplets is governed by the injector performance, and a typical slurry droplet may consist of many parent coal particles. The slurry droplet may undergo many different processes depending on the history of heating rates to which a particle is

subjected; these may include swelling under simultaneous or sequential vaporization of water and coal gaseous products, shattering of droplet into parent coal particles or even smaller particles, or fusion of porous char and ash particles. The model adopted here is the most simplistic one, which will be replaced by a more realistic model in the future. We assume that water vapor and coal devolatilization occur in a sequential process, with each droplet consisting of a single coal particle and a corresponding mass of water. Hence the spray size distribution is dictated by the original coal particle size distribution assumed. The initial step in the heating of the droplet is to increase particle temperature to the saturation temperature of water. This is followed by the water vaporization at the constant particle temperature until the particle is dry. Once the particle is dried it behaves like a dry coal particle. The sequential vaporization model has been found to be adequate for the case of coal water slurry turbulent diffusion flames.(10)

Gaseous Combustion Model

The original version of INTERN incorporated a two step reaction scheme for which differential transport governing the evolution of the mixture fraction f, mass fraction of unburned fuel m_{fu}; and mass fraction of CO, m_{CO}, were solved. Concentrations of other reactants including m_{O2} as well as equilibrium combustion products (M_{CO2}, m_{H2O}, m_{N2}, etc.) were obtained via algebraically formulated balance expressions.

To represent the combustion of two different kinds of volatiles and solids typicals of coal combustion, the following global mechanisms are postulated. The volatiles are assumed to combust to yield products CO and H_2 in the initial stage.

$$C_6H_6 + 3\ O_2 \xrightarrow{k_6} 6\ CO + 3\ H_2 \qquad (10)$$

$$C_6H_{12} + 3\ O_2 \xrightarrow{k_7} 6\ CO + 6\ H_2$$

The initial breakdown to CO and H_2 instead of CO_2 and H_2O is chosen to represent the fuel rich combustion situation of interest here. Subsequent oxidation of CO and H_2 are given by

$$CO + 1/2\ O_2 \underset{k_{8b}}{\overset{k_{8f}}{\rightleftharpoons}} CO_2 \qquad (11)$$

$$CO + 1/2\ O_2 \underset{k_{9b}}{\overset{k_{9f}}{\rightleftharpoons}} H_2O$$

Empirical rate constants k_6 to k_9 are required for finite rate kinetics. Reverse rate constants k_{8b} and k_{9b} are calculated from equilibrium considerations. For turbulent flows, the effective reaction rates are calculated from the eddy breakup model(11). In the absence of rate constants, the assumption of fast chemistry is invoked and all rates are limited by the turbulent mixing rates.

RESULTS AND DISCUSSION

A number of cases were computed for the toroidal vortex combustor geometry of interest. The combustor configuration, and the inlet air flow conditions have been kept constant throughout these computations. The initial conditions are summarized in Table 1. The composition and size distribution of fuel have been varied parametrically to examine its influence on the flow field. The range of variations for the variables are summarized in Table 2. In all the computations reported here, it is assumed that the tip of the coal injector is located at the center of the air jet and in the plane of the combustor wall. Coal particles are assumed to leave the injector at surrounding air velocity, but at room temperature, and the mass flux of carrier gas is assumed negligible compared to the coal mass flux.

The computations were performed on a grid of 37 x 16 x 9 nodes by finite difference algorithm of INTERN code. The iterations were carried out until the absolute sum of mass residuals was below a few percent. A typical set of velocity vector plots is shown in Fig. 2. The results for the injector plane ($k = 5$) show the existence of the jet directed towards the centerline. This jet broadens as it approaches the centerline and changes into a wall directed jet which curves along the walls of the combustor dome and escapes the injector plane by flowing around the initial jet. A circular vortex is seen to exist in the left hand corner of the combustor in each plane.

The typical set of calculated trajectories for the pulverized coal particles are shown in Fig. 3. A total of eight different size groups were selected such that the mass fraction in each size group is uniform. The mass weighted mean diameter for the distribution is 50 μm which roughly corresponds to 80 percent minus 200 mesh. In the computations, the particles are injected at the injector plane and their trajectories are followed until one of the three conditions is met: (i) particle combusts and is converted to an ash particle, at which time it is removed from further consideration, (ii) the particle hits the wall, or (iii) particle exits the combustor.

The fate of the particle hitting the wall depends on the wall boundary conditions. If walls are slagging then a particle is captured by the slag, follow the slag and in the process react through pyrolysis or a char burning mechanism. Since in the present work details of slag wall layer flow are not resolved, two limiting cases of particle wall interaction are considered. In the first case it is assumed that any particle hitting wall is completely lost from further consideration, while in the second case it is assumed that a particle hitting the wall is completely decomposed into gaseous fuel at the constant temperature. The latter process will be approached in the limit of extremely hot and sticky slag of negligible velocity, so that all volatilization will occur in the vicinity of the impact point. Since in most cases of practical interest, the design should ensure maximum burning in suspension, details of wall particle interaction may not be critical to combustion stability and flow field structure. However, wall reaction can contribute extensively to combustion of large coal particles. They ordinarily dominate residence time requirements for pure suspension combustion, and are most effectively combusted via wall reaction, which effectively provides extended residence time. In terms of fuel energy utilization, this mechanism is most attractive under reducing flow conditions.

In the case of dry pulverized coal (Case 1) with a mass mean particle diameter of 50 μm, approximately 81 percent of the fuel is utilized before particles hit the wall. If the fuel is substituted with a coal water mixture containing 30 percent water (Case 2) but otherwise the same size distribution as the dry coal, the fraction of fuel utilized is slightly increased to 86 percent. The slight increase in the fuel utilization may possibly be due

to the increased contribution from the gasification rate. The overall characteristics of the flow are unchanged, and there is a slight decrease in the temperature levels. Particles up to 23 μm are completely converted to ash in less than 34 ms, while larger particles only react partially before hitting the wall. The presence of water in coal alone does not adversely affect the combustion process, and there is slight evidence to suggest a beneficial effect possibly due to increased gasification of the char (see Equation 5).

The combustion process is more strongly dependent on the initial size distribution. Reducing the mass mean size from 50 μm (80 percent minus 200 mesh) to 33 μm (80 percent minus 325 mesh) results in increase of the fraction utilized from 86 percent to 94 percent (Case 3). In many coal water slurry applications, as discussed before, the size distribution of droplets is governed by the injector performance. If it is assumed that the injector produces practically monosized droplets of 33 μm diameter (Case 4), then the fraction of fuel utilized is dramatically reduced to 58 percent. Thus, as is well known, size distribution plays an important role in the combustion process. In the presence of a typical broad size distribution, fine particles release energy to increase the temperature level so that a 33 μm droplet is 70 percent utilized before it hits the wall, while in the presence of monosized droplets, a 33 μm droplet is 56 percent utilized.

If one assumes that a droplet is utilized completely as it hits the wall (Case 5) then by definition fuel is completely converted to gaseous fuel. In all the cases examined here, the combustor is operated fuel rich and utilization of O_2 is complete. Even when the fuel is not completely combusted, the combustor outflow is devoid of any oxygen. The volatiles released in the pyrolysis phase are of C_6H_{12} and C_6H_6 type, and some uncombusted volatiles (up to 2 percent by weight) are predicted. The presence of uncombusted volatiles may be due to the incomplete turbulent mixing of the volatiles or due to the inadequacy of the model which lacks the kinetic route for the dissociation or sasification of gaseous fuel to CO and H_2.

The combustor exit conditions are relatively insensitive to the initial size distribution and composition of fuel. The detailed temperature and species distributions inside the combustor, however, are strongly sensitive to the size distribution. As an example the temperature and CO mass fraction contours in the injector plane are compared in Figs. 4 and 5, respectively.

The ability of the code to compute complex three-dimensional combustor flow fields has been demonstrated. The purpose of the model work was specifically as a design tool for exploration of combustor geometry, sizing, and fuel choices. It was successful and useful in that regard. The model has given reasonable qualitative prediction of the toroidal vortex flow field under cold flow conditions.[12] Also, as the test data become available from the combustor development program, quantitative comparisons will be made and the model revised to improve physical assumptions.

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References

(1) Lockwood, F. C., Rizvi, S.M.A., Lee, G. K. and Whaley, H., Twentieth International Symposium on Combustion, pp 513-522, Combustion Institute, Pittsburgh, 1984.

(2) Truelove, J. S., pp 523-530, ibid.

(3) Smoot, L. D., and Smith, P. J., Coal Combustion and Gasification, Plenum Press, New York, 1985.

(4) Swithenbank, J., Turan, A., Felton, P. G., and Spalding, D. B., AGARD Conference Proceeding No. 275 on Combustor Modelling, 1979.

(5) Turan, A., A Three-Dimensional Mathemetical Model for Gas Turbine Combustors, Ph.D. Thesis, University of Sheffield, 1978.

(6) Bruce, T. W., Mongia, H. C., and Reynolds, R. S. Combustor Design Criteria Validation, Vol. III, USARTL-TR-78-55, AVRAD Com, Fort Eustis, Virginia, March 1979.

(7) Kobayashi, H., Howard, J. B., and Sarofim, A. F., Eighteenth International Symposium on Combustion, p 411, The Combustion Institute, Pittsburgh, 1977.

(8) Field, M. A., Combust Flame, 14 237 (1970).

(9) Stickler, D. B., Becker, F. E., and Ubhayakar, S. K., AIAA Paper No. 79-0298.

(10) Srinivasachar, S., Farmayan, W. F., and Beer, J. M., Second European Conference on Coal Liquid Mixtures, 16-18 Sept., 1985, London.

(11) Magnussen, B.F., and Hertager, B. H., in Sixteenth International Symposium on Combustion, p 719, The Combustion Institute, Pittsburgh, 1977.

(12) Chatwani, A.U., and Turan, A. Submitted to Western States Meeting of the Combustion Institute, Salt Lake City, Utah, March 1988.

TABLE 1

COMBUSTOR CONFIGURATION AND INITIAL CONDITIONS

Combustor Diameter	0.35 m
Injector-Dome Length	0.43 m
No. of Injectors	4
Injection Angle	60
Air Flow Rate	0.37 kg/s
Air Injection Velocity	70 m/s
Air Injection Temp.	617 K
Air Pressure	6 atm

TABLE 2

INITIAL CONDITIONS FOR FUEL COMPOSITION

	Case 1	Case 2	Case 3	Case 4	Case 5
$\dot{m}_{fuel}$	0.051	0.073	0.073	0.073	0.073
$\dot{m}_{water}/\dot{m}_{fuel}$	0.0	0.3	0.3	0.3	0.3
$\dot{m}_{daf}/\dot{m}_{fuel}$	0.95	0.665	0.665	0.665	0.665
d	50 μ	50 μ	33 μ	33 μ	33 μ
f(d)	exp (d/d)	exp (d/d)	exp (d/d)	δ (d/d)	δ (d/d)
ø	1.3	1.3	1.3	1.3	1.3
Particle/Wall Interaction Model	1	1	1	1	2

(1) Particle Capture, no vaporization
(2) Particle Capture, Complete vaporization

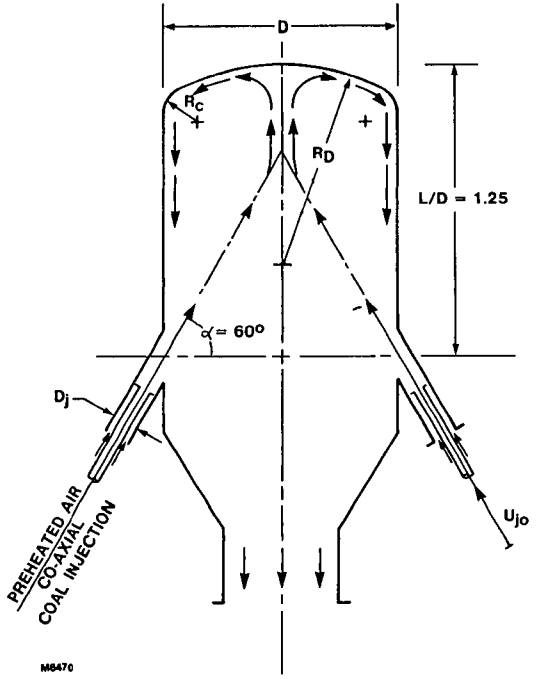

Figure 1 Schematic of Combustor Geometry

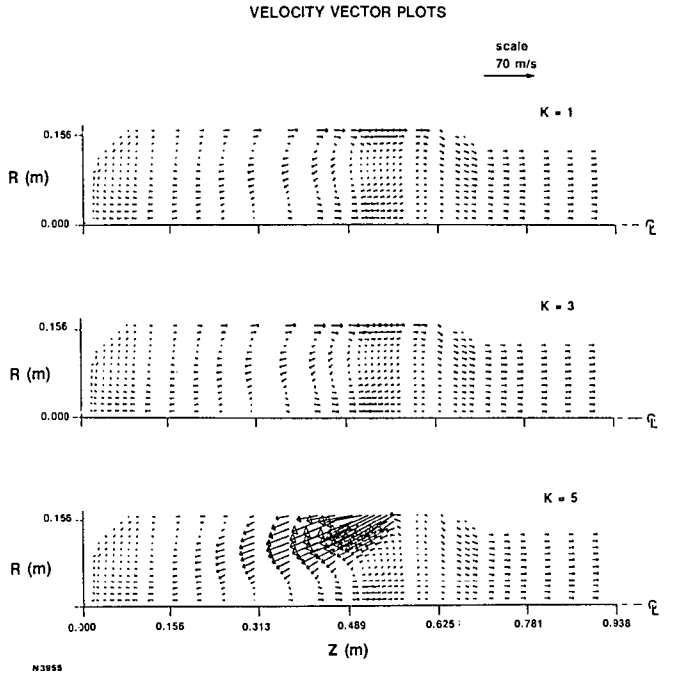

Figure 2 Typical Velocity Vector Plots in r-z Plane

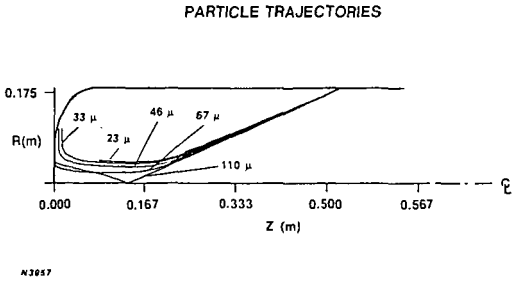

Figure 3 Typical Particle Trajectories in r-z Plane

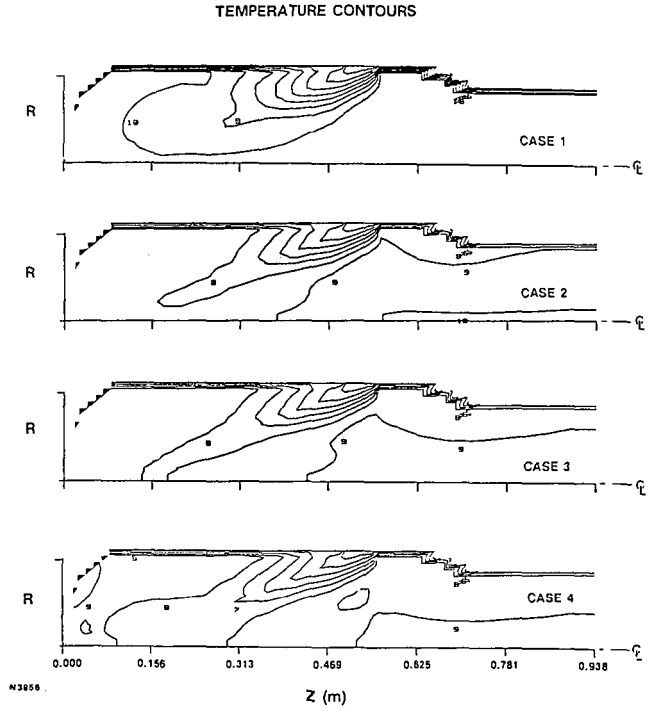

Figure 4 Computed Temperature Contour Plots.
Contour 1 = 300K, Contour 11 = 2800K, increment = 250K

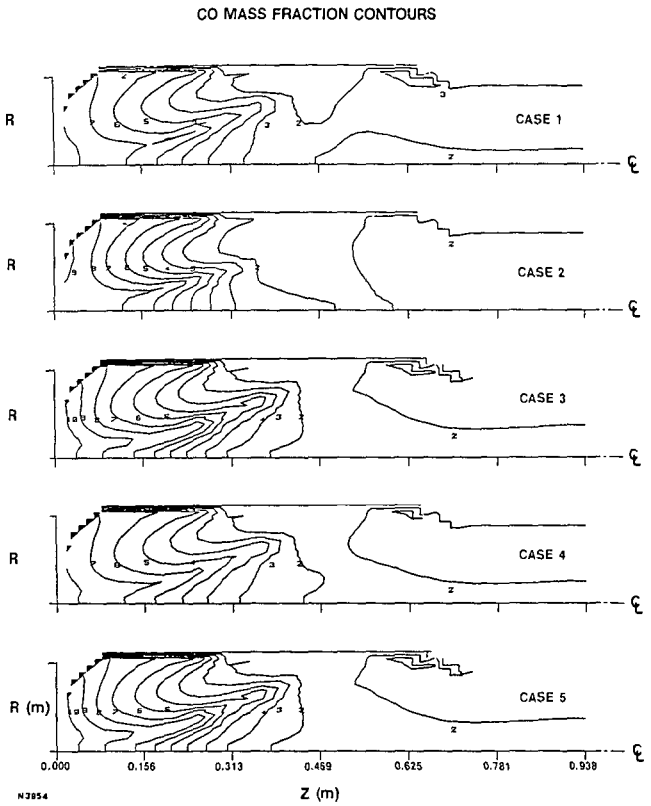

Figure 5 Computed CO Mass Fraction Contour Plots.
Contour 1 = 0, Contour 11 = 0.4, increment = 0.04